# EAST Search History

| Ref # | Hits | Search Query | DBs | Default Operator | Plurals | Time Stamp |
|---|---|---|---|---|---|---|
| L1 | 4 | ("20030060459"\|"20030216434"\|"6011052"\|"6706712").PN. | US-PGPUB; USPAT | OR | ON | 2006/12/13 13:24 |
| L2 | 4 | ("20040110736"\|"20040235836"\|"20040235835"\|"20050043392").PN. | US-PGPUB; USPAT | OR | ON | 2006/12/13 13:43 |
| L3 | 1 | ("20030171218").PN. | US-PGPUB; USPAT | OR | ON | 2006/12/13 15:31 |
| L4 | 885 | 548/518.ccls. | US-PGPUB; USPAT | OR | ON | 2006/12/13 15:31 |

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJRK1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page URLs for STN Seminar Schedule - N. America |
| NEWS 2 | | "Ask CAS" for self-help around the clock |
| NEWS 3 | AUG 09 | INSPEC enhanced with 1898-1968 archive |
| NEWS 4 | AUG 28 | ADISCTI Reloaded and Enhanced |
| NEWS 5 | AUG 30 | CA(SM)/CAplus(SM) Austrian patent law changes |
| NEWS 6 | SEP 11 | CA/CAplus enhanced with more pre-1907 records |
| NEWS 7 | SEP 21 | CA/CAplus fields enhanced with simultaneous left and right truncation |
| NEWS 8 | SEP 25 | CA(SM)/CAplus(SM) display of CA Lexicon enhanced |
| NEWS 9 | SEP 25 | CAS REGISTRY(SM) no longer includes Concord 3D coordinates |
| NEWS 10 | SEP 25 | CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine |
| NEWS 11 | SEP 28 | CEABA-VTB classification code fields reloaded with new classification scheme |
| NEWS 12 | OCT 19 | LOGOFF HOLD duration extended to 120 minutes |
| NEWS 13 | OCT 19 | E-mail format enhanced |
| NEWS 14 | OCT 23 | Option to turn off MARPAT highlighting enhancements available |
| NEWS 15 | OCT 23 | CAS Registry Number crossover limit increased to 300,000 in multiple databases |
| NEWS 16 | OCT 23 | The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded |
| NEWS 17 | OCT 30 | CHEMLIST enhanced with new search and display field |
| NEWS 18 | NOV 03 | JAPIO enhanced with IPC 8 features and functionality |
| NEWS 19 | NOV 10 | CA/CAplus F-Term thesaurus enhanced |
| NEWS 20 | NOV 10 | STN Express with Discover! free maintenance release Version 8.01c now available |
| NEWS 21 | NOV 13 | CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role |
| NEWS 22 | NOV 20 | CAS Registry Number crossover limit increased to 300,000 in additional databases |
| NEWS 23 | NOV 20 | CA/CAplus to MARPAT accession number crossover limit increased to 50,000 |
| NEWS 24 | NOV 20 | CA/CAplus patent kind codes will be updated |
| NEWS 25 | DEC 01 | CAS REGISTRY updated with new ambiguity codes |
| NEWS 26 | DEC 11 | CAS REGISTRY chemical nomenclature enhanced |

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

| | |
|---|---|
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS IPC8 | For general information regarding STN implementation of IPC 8 |
| NEWS X25 | X.25 communication option no longer available |

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:26:24 ON 13 DEC 2006

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 10:26:36 ON 13 DEC 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1
DICTIONARY FILE UPDATES: 12 DEC 2006 HIGHEST RN 915277-53-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

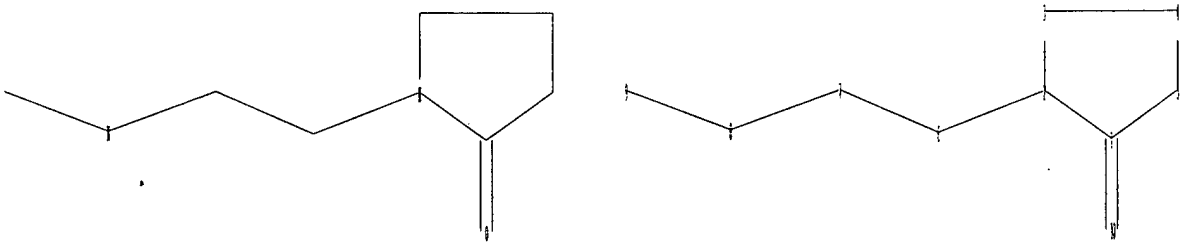
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 1.str



chain nodes :
6 7 8 9 10
ring nodes :
1 2 3 4 5
chain bonds :

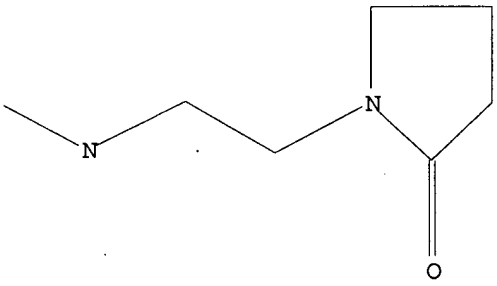
10776586.trn

1-10 2-6 6-7 7-8 8-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-10 2-3 2-6 3-4 4-5 7-8 8-9
exact bonds :
6-7

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR




Structure attributes must be viewed using STN Express query preparation.

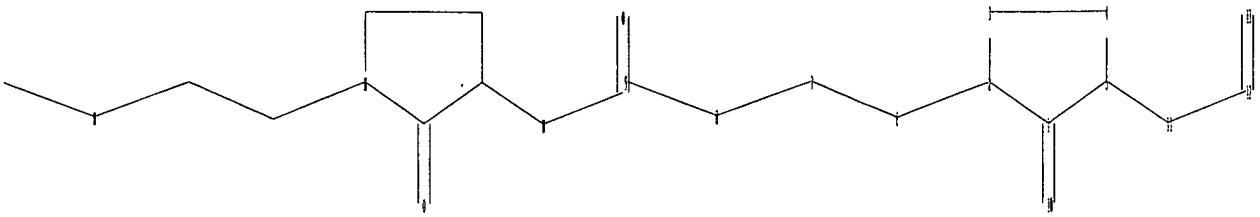
=> l1
SAMPLE SEARCH INITIATED 10:26:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2466 TO ITERATE

81.1% PROCESSED 2000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 46342 TO 52298
PROJECTED ANSWERS: 11745 TO 14837

L2 50 SEA SSS SAM L1

=>
Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 2.str

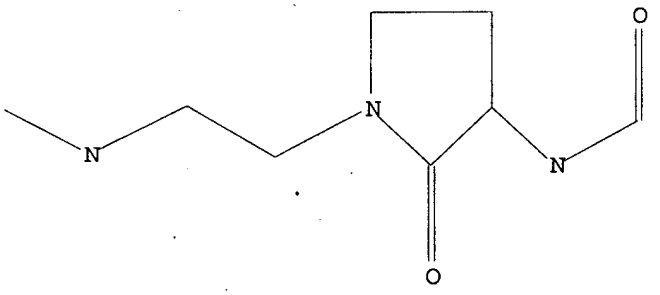


chain nodes :
6 7 8 9 10 11 12 13
ring nodes :
1 2 3 4 5
chain bonds :
1-10 2-6 5-11 6-7 7-8 8-9 11-12 12-13
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-10 2-3 2-6 3-4 4-5 5-11 7-8 8-9 11-12 12-13
exact bonds :
6-7

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS

L3 STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3 STR




Structure attributes must be viewed using STN Express query preparation.

=> l3
SAMPLE SEARCH INITIATED 10:27:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 79 TO ITERATE

100.0% PROCESSED 79 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          1047 TO     2113
PROJECTED ANSWERS:              592 TO     1448

L4           50 SEA SSS SAM L3

=> l3 full
FULL SEARCH INITIATED 10:27:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1291 TO ITERATE

100.0% PROCESSED     1291 ITERATIONS                                874 ANSWERS
SEARCH TIME: 00.00.01

L5           874 SEA SSS FUL L3

=> file medline caplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     167.38     167.59

FILE 'MEDLINE' ENTERED AT 10:27:48 ON 13 DEC 2006

FILE 'CAPLUS' ENTERED AT 10:27:48 ON 13 DEC 2006
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COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

=> l5
L6           300 L5

=> dup rem l6
PROCESSING COMPLETED FOR L6
L7            284 DUP REM L6 (16 DUPLICATES REMOVED)

=> file reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      18.33     185.92

FILE 'REGISTRY' ENTERED AT 10:28:07 ON 13 DEC 2006
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STRUCTURE FILE UPDATES:   12 DEC 2006  HIGHEST RN 915277-53-1
DICTIONARY FILE UPDATES:  12 DEC 2006  HIGHEST RN 915277-53-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

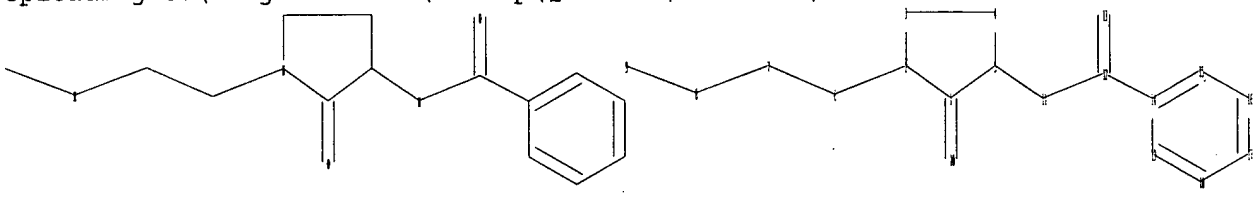
  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
```

predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 3.str

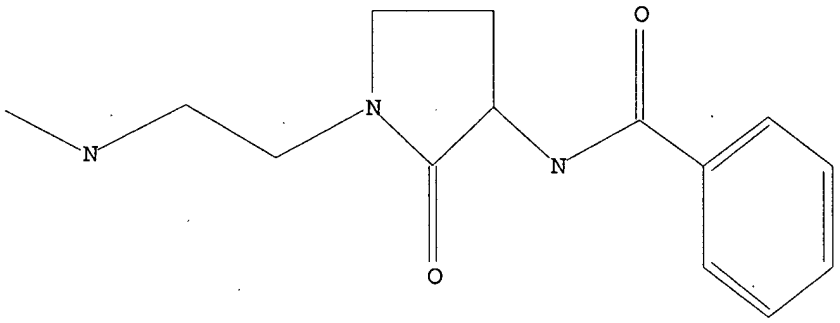


chain nodes :
6 7 8 9 10 11 12 13
ring nodes :
1 2 3 4 5 14 15 16 17 18 19
chain bonds :
1-10 2-6 5-11 6-7 7-8 8-9 11-12 12-13 12-14
ring bonds :
1-2 1-5 2-3 3-4 4-5 14-15 14-19 15-16 16-17 17-18 18-19
exact/norm bonds :
1-2 1-5 1-10 2-3 2-6 3-4 4-5 5-11 7-8 8-9 11-12 12-13
exact bonds :
6-7 12-14
normalized bonds :
14-15 14-19 15-16 16-17 17-18 18-19

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom
19:Atom

L8 STRUCTURE UPLOADED

=> d
L8 HAS NO ANSWERS
L8 STR




Structure attributes must be viewed using STN Express query preparation.

```
=> l8
SAMPLE SEARCH INITIATED 10:28:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        21 TO ITERATE

100.0% PROCESSED        21 ITERATIONS                                  1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          146 TO      694
PROJECTED ANSWERS:               1 TO       80

L9             1 SEA SSS SAM L8

=> l8 full
FULL SEARCH INITIATED 10:28:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       394 TO ITERATE

100.0% PROCESSED      394 ITERATIONS                                 23 ANSWERS
SEARCH TIME: 00.00.01

L10           23 SEA SSS FUL L8

=> file medline caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   166.94     352.86

FILE 'MEDLINE' ENTERED AT 10:28:52 ON 13 DEC 2006

FILE 'CAPLUS' ENTERED AT 10:28:52 ON 13 DEC 2006
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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=> l10
L11           8 L10

=> dup rem l11
PROCESSING COMPLETED FOR L11
L12            8 DUP REM L11 (0 DUPLICATES REMOVED)
```

=> d ibib abs hitstr 1-8

L12 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:701971 CAPLUS
DOCUMENT NUMBER: 141:225303
TITLE: Preparation of N-[(benzylaminomethyl)alkyl]-2-(acylamino)pyrrolidinones as modulators of chemokine receptor activity
INVENTOR(S): Carter, Percy; Voss, Matthew E.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 140 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004071449 | A2 | 20040826 | WO 2004-US4151 | 20040211 |
| WO 2004071449 | A3 | 20050106 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 2004186143 | A1 | 20040923 | US 2004-776586 | 20040211 |
| PRIORITY APPLN. INFO.: | | | US 2003-446976P | P 20030212 |

OTHER SOURCE(S): MARPAT 141:225303
GI

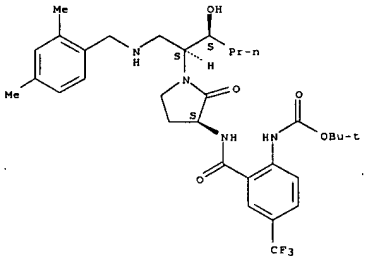
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Lactams I [A = (CHR14)n; E = CH2CH2, CH:CH; Q = O, S; R1, R2 = (un)substituted aryl or heteroaryl containing N, O, or S atoms; R3, R6, R7, R8, R9, R10, R11, R12 = H, (un)substituted hydroxyalkyl, mercaptoalkyl, alkoxyalkyl, sulfinylalkyl, sulfonylalkyl, etc.; R13, R14 = H, (un)substituted alkyl; R16, R17 = H, (un)substituted alkyl, cycloalkyl; X = NR17, CHR16NR17; Z = bond, (un)substituted aminocarbonyl, carbonylamino, aminothiocarbonyl, aminosulfonyl, aminosulfonylamino, etc.; m, q = 0-1; n = 0-3; p = 0-1], particularly the N-[(benzylaminomethyl)alkyl]-2-(acylamino)pyrrolidinones II [R20 = 3-(F3C)C6H4, 3-(F3C)C6H4NH, 2-(BocNH)-5-(F3C)C6H3, 2-H2N-5-(F3C)C6H3, 3-H2N-5-(F3C)C6H3] and III, are prepared as chemokine receptor modulators for the treatment of diseases such as rheumatoid arthritis, multiple sclerosis, atherosclerosis, asthma, restenosis, and cancer and diseases related to organ transplantation. (S,S)-CbzNHCH2CH(NHBoc)CH(OH)C.tplbond.CMe is deprotected with trifluoroacetic acid and acylated with Boc-methionine with BOP; methylation of the thiomethyl group with Me iodide, cyclization with sodium hydride, hydrogenolysis of the Cbz protecting group and redn. of the alkyne, reductive amination of the free amine with 2,4-dimethylbenzaldehyde and reprotection of the secondary amino group with a Cbz moiety, Boc deprotection, BOP-mediated acylation with 3-trifluoromethylbenzoic acid, and hydrogenolysis of the Cbz protecting group yields II [R20 = 3-(F3C)C6H4]. Compds. of the invention inhibit MCP-1 binding to human peripheral blood mononuclear cells by 50% at concn. of <20μM (no data).

IT 747149-84-4P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzylaminomethylalkyl acylaminopyrrolidinones as cytokine receptor modulating agents for the treatment of diseases such as rheumatoid arthritis, multiple sclerosis, atherosclerosis, asthma, restenosis, and cancer)

RN 747149-84-4 CAPLUS
CN Carbamic acid, [2-[[[(3S)-1-[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]-2-oxo-3-pyrrolidinyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

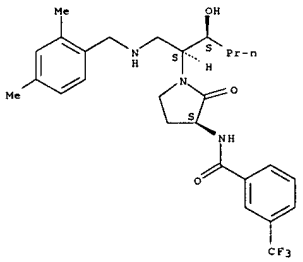
Absolute stereochemistry.



IT 747149-73-1P 747149-88-8P 747149-95-7P
747150-00-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzylaminomethylalkyl acylaminopyrrolidinones as cytokine receptor modulating agents for the treatment of diseases such as rheumatoid arthritis, multiple sclerosis, atherosclerosis, asthma, restenosis, and cancer)

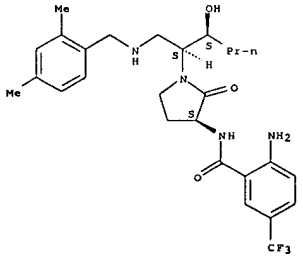
RN 747149-73-1 CAPLUS
CN Benzamide, N-[(3S)-1-[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]-2-oxo-3-pyrrolidinyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 747149-88-8 CAPLUS
CN Benzamide, 2-amino-N-[(3S)-1-[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]-2-oxo-3-pyrrolidinyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

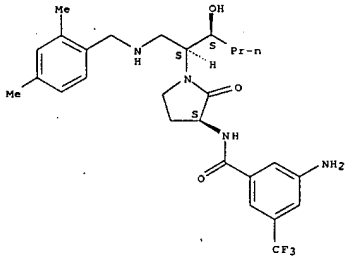
Absolute stereochemistry.



RN 747149-95-7 CAPLUS

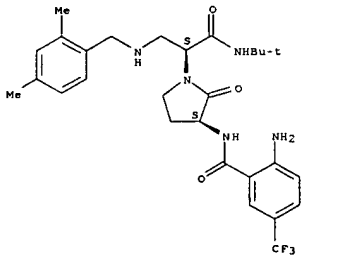
L12 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Benzamide, 3-amino-N-[(3S)-1-[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]-2-oxo-3-pyrrolidinyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 747150-00-1 CAPLUS
CN 1-Pyrrolidineacetamide, 3-[[2-amino-5-(trifluoromethyl)benzoyl]amino]-N-(1,1-dimethylethyl)-α-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-oxo-, (αS,3S)- (9CI) (CA INDEX NAME)

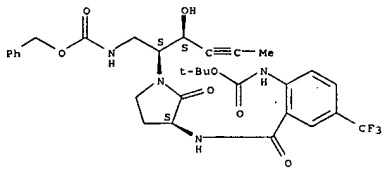
Absolute stereochemistry.



IT 747150-20-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzylaminomethylalkyl acylaminopyrrolidinones as cytokine

L12 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
receptor modulating agents for the treatment of diseases such as rheumatoid arthritis, multiple sclerosis, atherosclerosis, asthma, restenosis, and cancer)
RN 747150-20-5 CAPLUS
CN Carbamic acid,
[(2S,3S)-2-[(3S)-3-[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]-2-oxo-1-pyrrolidinyl]-3-hydroxy-4-hexynyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

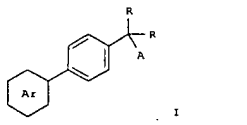


L12 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:695961 CAPLUS
DOCUMENT NUMBER: 137:216961
TITLE: Preparation of bisaryl derivatives having FSH receptor modulatory activity
INVENTOR(S): Guo, Tao; Ho, Koc-Kan; McDonald, Edward; Dolle, Roland Ellwood; Saionz, Kurt W.; Kultgen, Steven G.; Liu, Ruiyan; Dong, Guizhen; Geng, Peng; Adang, Anton Egbert Peter; Van Straten, Nicole Corine Renee
PATENT ASSIGNEE(S): Pharmacopeia, Inc., USA
SOURCE: PCT Int. Appl., 167 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2002070493 | A1 | 20020912 | WO 2002-US3777 | 20020118 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2434184 | AA | 20020912 | CA 2002-2434184 | 20020118 |
| EP 1351941 | A1 | 20031015 | EP 2002-717403 | 20020118 |
| EP 1351941 | B1 | 20040929 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR | | | | |
| AT 277913 | E | 20041015 | AT 2002-717403 | 20020118 |
| JP 2005505496 | T2 | 20050224 | JP 2002-569813 | 20020118 |
| US 2004152703 | A1 | 20040805 | US 2003-623640 | 20030721 |
| US 6900213 | B2 | 20050531 | | |
| PRIORITY APPLN. INFO.: | | | EP 2001-200194 A | 20010119 |
| | | | WO 2002-US3777 W | 20020118 |

OTHER SOURCE(S): MARPAT 137:216961
GI

L12 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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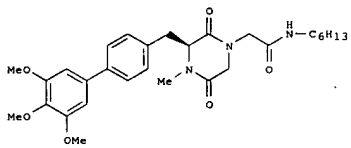
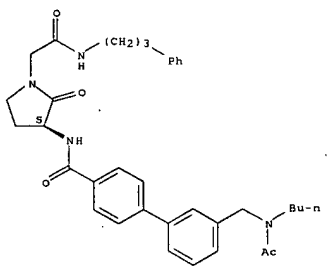


II

AB Title compds. I [R,R = H/H, O, H/Me, H/OH, H/CN; A = pyridazindione, etc.;
Ar = (un)substituted phenyl] were prepared For example, a photolabile-supported 1-hexylamine derivative was acylated with (3S)-1-carboxymethyl-3-(4-iodobenzyl)-4-methyl-2,5-dioxopiperazine (preparation
given) followed by coupling of the resulting aryl iodide with 3,4,5-trimethoxybenzeneboronic acid (DME/EtOH, Pd2(dba)3, Ph3As, CsF). The resulting resin was irradiated at 365 nm at 50° (MeOH/TFA) to yield II. II had EC50 < 10 μM for the FSH receptor. I are useful in the treatment for the control of fertility, for contraception or for treatment of hormone-dependent disorders.
IT 457614-55-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(FSH receptor modulator; preparation of pyridazinedione-substituted bisaryl
derivs. having FSH receptor modulatory activity)
RN 457614-55-0 CAPLUS
CN 1-Pyrrolidineacetamide,
3-[[[3'-[(acetylbutylamino)methyl][1,1'-biphenyl]-4-yl]carbonyl]amino]-2-oxo-N-(3-phenylpropyl)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

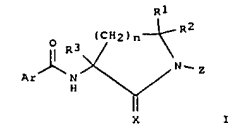
L12 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:824216 CAPLUS
DOCUMENT NUMBER: 134:4857
TITLE: Preparation of 3-acylamino-3-methylpyrrolidin-2-ones and analogs as metabotropic glutamate receptor antagonists
INVENTOR(S): Clark, Barry Peter; Cwi, Cynthia Lynn; Harris, John Richard; Kingston, Ann Elizabeth; Scott, William Leonard
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2000069816 | A1 | 20001123 | WO 2000-US8223 | 20000517 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1183238 | A1 | 20020306 | EP 2000-930094 | 20000517 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |

PRIORITY APPLN. INFO.: US 1999-134410P P 19990517
WO 2000-US8223 W 20000517

OTHER SOURCE(S): MARPAT 134:4857
GI

L12 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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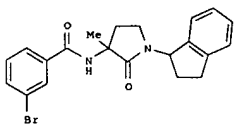


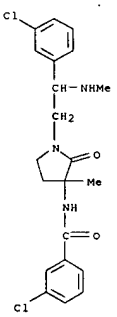
II

AB The title compds. (I) [wherein n = 0-2; X = O, S, NH, or NOH; R1 and R2 = independently H, CN, CO2R, CONHR, alkyl, or tetrazole; or R1 and R2 together = :O; R = H or alkyl; R3 = (cyclo)alkyl, alkenyl, CH2OH, alkoxymethyl, or CO2H; Ar = (un)substituted (hetero)aromatic group; Z = (un)substituted indanyl, indenyl, phenylalkyl, phenylcyclopropyl, or CH2BHet; B = CHR, CR2, alkyl, CO, CHOH, CH2O, CH:CH, CH2CO, CH2S, CH2S(O), CH2SO2, CHCO2R, or CHNR2; Het = heterocycle] were prepared by conventional and solution phase combinatorial methods for the treatment or prevention of a physiol. disorder associated with an excess of stimulation of the human Group I metabotropic glutamate receptors, especially those designated as mGluR5. Examples include syntheses and phys. data for approx. 140 compds., description of bioassays with data summaries, and 8 pharmaceutical formulations employing I. Thus, (R,R)-II was prepared by reductive amination of N-(3-bromobenzoyl)-α-(2-oxoethyl)alanine (preparation given) with R-(-)-1-aminoindane in the presence of NaBH4 in MeOH followed by spontaneous cyclization to the lactam. When mGluR5 expressing cell lines were used, representative compds. of the invention generated IC50 values of ≤ 30 μM in a phosphoinositide assay and resulted in ≥ 70% inhibition at concns. of 30 μM in a calcium flux assay. I are useful in the treatment of neurodegenerative conditions and pain (no data).

IT 308817-13-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

L12 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(prepn. of 3-acylamino-3-methylpyrrolidin-2-ones and analogs by conventional and soln. phase combinatorial methods as metabotropic glutamate receptor antagonists)

RN 308817-13-2 CAPLUS
CN Benzamide, 3-chloro-N-[1-[2-(3-chlorophenyl)-2-(methylamino)ethyl]-3-methyl-2-oxo-3-pyrrolidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

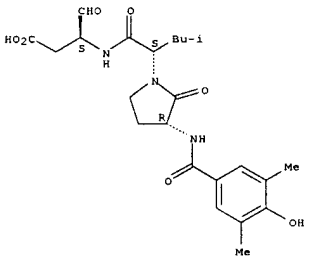
L12 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:613942 CAPLUS
DOCUMENT NUMBER: 131:243593
TITLE: Preparation of peptides as inhibitors of caspases
INVENTOR(S): Wannamaker, Marion W.; Bemis, Guy W.; Charifson, Paul S.; Lauffer, David J.; Mullican, Michael D.; Murcko, Mark A.; Wilson, Keith P.; Janetka, James W.; Davies, Robert J.; Grillot, Anne-Laure; Shi, Zhan; Forster, Cornelia J.
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 297 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9947545 | A2 | 19990923 | WO 1999-US5919 | 19990319 |
| WO 9947545 | A3 | 19991125 | | |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2324226 | AA | 19990923 | CA 1999-2324226 | 19990319 |
| AU 9930986 | A1 | 19991011 | AU 1999-30986 | 19990319 |
| AU 769033 | B2 | 20040115 | | |
| BR 9909660 | A | 20001121 | BR 1999-9660 | 19990319 |
| EP 1064298 | A2 | 20010103 | EP 1999-912662 | 19990319 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |
| HU 200103575 | A2 | 20020228 | HU 2001-3575 | 19990319 |
| JP 2002506878 | T2 | 20020305 | JP 2000-536738 | 19990319 |
| TR 200103406 | T2 | 20020621 | TR 2001-200103406 | 19990319 |
| NZ 506963 | A | 20031031 | NZ 1999-506963 | 19990319 |
| NZ 528282 | A | 20050527 | NZ 1999-528282 | 19990319 |
| TW 243828 | B1 | 20051121 | TW 1999-88104386 | 19990319 |
| RU 2274642 | C2 | 20060420 | RU 2000-126298 | 19990319 |
| ZA 2000004652 | A | 20020205 | ZA 2000-4652 | 20000905 |
| NO 2000004546 | A | 20001109 | NO 2000-4546 | 20000912 |
| US 6531474 | B1 | 20030311 | US 2000-665503 | 20000919 |
| BG 104863 | A | 20010430 | BG 2000-104863 | 20001016 |
| US 2003232986 | A1 | 20031218 | US 2002-314103 | 20021206 |
| AU 2003255217 | A1 | 20031113 | AU 2003-255217 | 20031022 |
| JP 2006206600 | A2 | 20060810 | JP 2006-75461 | 20060317 |

PRIORITY APPLN. INFO.:
US 1998-78770P A1 19980319
AU 1999-30986 A3 19990319
JP 2000-536738 A3 19990319
WO 1999-US5919 W 19990319
US 2000-665503 A3 20000919

L12 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 131:243593
AB Peptides R1NR2XCONR4CR52CONHY [Y = CH(CHO)CH2(CH2)mCOR7, (m = 0 or 1 and R7 = OH or ester, NHOH) or cyclic lactol derivative when R7 is OH; X = CR32 or NR3 (R3 = H, an amino acid side chain, alkyl, cycloalkyl, aryl, etc.); R1 = H, R8, COR8, COCOR8, SO2R8, SOR8, CO2R8, CONHR8, SO2NHR8, SONHR8, COCONHR8, COCH:CHR8, etc. (R8 = alkyl, cycloalkyl, aryl, etc.); R2 = H or R2 and R3 may form a ring; R4 = H and R5 = H, amino acid side chain, R8, etc. or R4 and R5 may form a ring] were prepared as inhibitors of caspases. Thus, p-AcNHC6H4CO-L-Val-L-Pro-NHCH(CHO)CH2CO2H-(S) was prepared by the solid-phase method and showed ki < 10 nm for inhibition of interleukin-1β converting enzyme (ICE, caspase-1).
IT 244132-96-5P 244132-97-6P 244132-99-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as inhibitors of caspases)
RN 244132-96-5 CAPLUS
CN Butanoic acid, 3-[[(2S)-2-[(3R)-3-[(4-hydroxy-3,5-dimethylbenzoyl)amino]-2-oxo-1-pyrrolidinyl]-4-methyl-1-oxopentyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

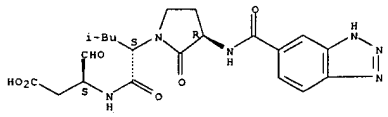
Absolute stereochemistry.



RN 244132-97-6 CAPLUS
CN Butanoic acid, 3-[[(2S)-2-[(3R)-3-[(1H-benzotriazol-5-ylcarbonyl)amino]-2-oxo-1-pyrrolidinyl]-4-methyl-1-oxopentyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

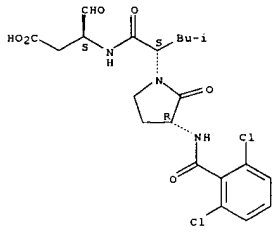
Absolute stereochemistry.

L12 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

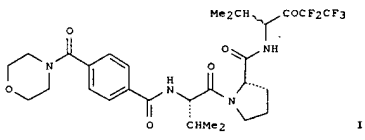


RN 244132-99-8 CAPLUS
CN Butanoic acid, 3-[[(2S)-2-[(3R)-3-[(2,6-dichlorobenzoyl)amino]-2-oxo-1-pyrrolidinyl]-4-methyl-1-oxopentyl]amino]-4-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



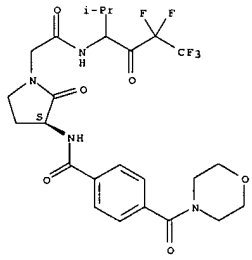
L12 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:430286 CAPLUS
DOCUMENT NUMBER: 129:41393
TITLE: Inhibition of Human Neutrophil Elastase. 4. Design, Synthesis, X-ray Crystallographic Analysis, and Structure-Activity Relationships for a Series of P2-Modified, Orally Active Peptidyl Pentafluoroethyl Ketones
AUTHOR(S): Cregge, Robert J.; Durham, Sherrie L.; Farr, Robert A.; Gallion, Steven L.; Hare, C. Michelle; Hoffman, Robert V.; Janusz, Michael J.; Kim, Hwa-Ok; Koehl, Jack R.; Mehdi, Shujaath; Metz, William A.; Peet, Norton P.; Pelton, John T.; Schreuder, Herman A.; Sunder, Shyam; Tardif, Chantal
CORPORATE SOURCE: Hoechst Marion Roussel Inc., Cincinnati, OH, 45215, USA
SOURCE: Journal of Medicinal Chemistry (1998), 41(14), 2461-2480
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

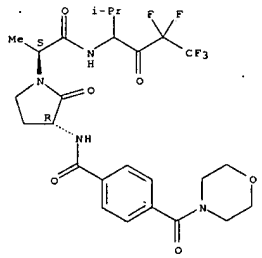
AB A series of P2-modified, orally active peptidic inhibitors of human neutrophil elastase (HNE) are reported. These pentafluoroethyl ketone-based inhibitors were designed using pentafluoroethyl ketone I (MDL 101,146) as a model. Rational structural modifications were made at the P3, P2, and activating group (AG) portions of I based on structure-activity relationships (SAR) developed from in vitro (measured Ki) data and information provided by modeling studies that docked inhibitor I into the active site of HNE. The modeling-based design was corroborated with X-ray crystallog. anal. of the complex between I and porcine pancreatic elastase (PPE) and subsequently the complex between I and HNE.
IT 208113-53-5P 208113-55-7P 208113-57-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of peptidyl pentafluoroethyl ketones as inhibitors of human neutrophil elastase)
RN 208113-53-5 CAPLUS
CN 1-Pyrrolidineacetamide, 3-[[4-(4-morpholinylcarbonyl)benzoyl]amino]-2-oxo-N-[3,3,4,4,4-pentafluoro-1-(1-methylethyl)-2-oxobutyl]-, (3S)- (9CI) (CA INDEX NAME)

L12 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.



RN 208113-55-7 CAPLUS
CN 1-Pyrrolidineacetamide, α-methyl-3-[[4-(4-morpholinylcarbonyl)benzoyl]amino]-2-oxo-N-[3,3,4,4,4-pentafluoro-1-(1-methylethyl)-2-oxobutyl]-, (αS,3R)- (9CI) (CA INDEX NAME)

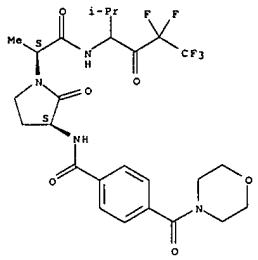
Absolute stereochemistry.



RN 208113-57-9 CAPLUS
CN 1-Pyrrolidineacetamide, α-methyl-3-[[4-(4-morpholinylcarbonyl)benzoyl]amino]-2-oxo-N-[3,3,4,4,4-pentafluoro-1-(1-methylethyl)-2-oxobutyl]-, (αS,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L12 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



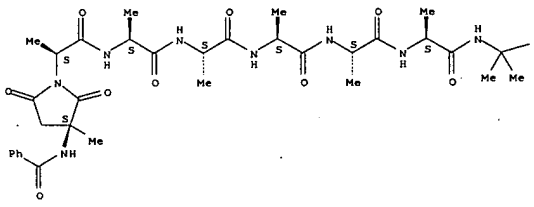
REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:646051 CAPLUS
DOCUMENT NUMBER: 127:307651
TITLE: Design and synthesis of novel nonpolar host peptides for the determination of the 310- and α-helix compatibilities of α-amino acid building blocks: an assessment of α,α-disubstituted glycines
AUTHOR(S): Obrecht, Daniel; Altorfer, Michael; Bohdal, Udo; Daly,
John; Huber, Walter; Labhardt, Alexander; Lehmann, Christian; Muller, Klaus; Ruffieux, Ruth; Schonholzer,
Peter; Spiegler, Clive; Zumbrunn, Cornelia
CORPORATE SOURCE: F. Hoffmann-La Roche AG, Pharma Research, Basel, CH-4070, Switz.
SOURCE: Biopolymers (1997), 42(5), 575-626
CODEN: BIPMAA; ISSN: 0006-3525
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The present work describes three novel nonpolar host peptide sequences that provide a ready assessment of the 310- and α-helix compatibilities of natural and unnatural amino acids at different positions of small- to medium-size peptides. The unpolar peptides containing
Ala, α-aminoisobutyric acid (Aib), and a C-terminal p-iodoanilide group were designed in such a way that the peptides could be rapidly assembled in a modular fashion, were highly soluble in solvent mixts. of triflouroethanol and H2 for CD and two-dimensional NMR analyses, and showed excellent crystallinity suited for x-ray structure anal. To validate this approach, 9-mer peptides, 12-mer peptides, and 10-mer peptides incorporating a series of optically pure cyclic and open-chain (R)- and (S)-α,α-disubstituted glycines were prepared These amino acids are known to significantly modulate the conformations of small
peptides. Based on x-ray structures, CD spectra recorded in acidic, neutral, and basic media and detailed 2D-NMR analyses, several interesting
conformational observations were made. Especially interesting results were
obtained using the convex constraint CD anal. proposed by Fasman, which allowed the determination of the relative content of 310- and α-helical conformations. These results were fully supported by the corresponding x-ray and 2D-NMR analyses. As a striking example, it was found that the (S)- and (R)-β-tetralin derived amino acids show excellent
α-helix stabilization, more pronounced than Aib and Ala. These novel reference peptide sequences should help establish a scale for natural and
unnatural amino acids concerning their intrinsic 310-and α-helix compatibilities at different positions of medium-sized peptides and thus improve the understanding of folding processes in peptides.
IT 197381-77-4P 197381-80-9P 197382-01-7P
197382-03-9P 197382-05-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(design and synthesis of novel nonpolar host peptides for determination of 310-

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
and α-helix compatibilities of disubstituted glycine building blocks)
RN 197381-77-4 CAPLUS
CN L-Alaninamide, N-[(2S)-2-[(3S)-3-(benzoylamino)-3-methyl-2,5-dioxo-1-pyrrolidinyl]-1-oxopropyl]-L-alanyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

PAGE 1-A



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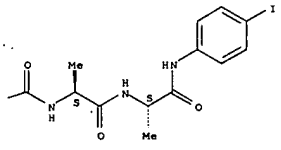
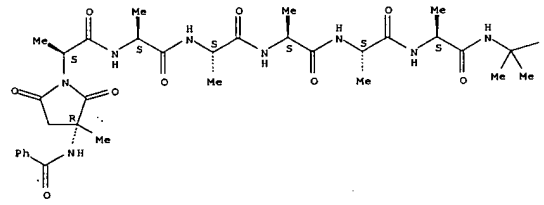


RN 197381-80-9 CAPLUS
CN L-Alaninamide, N-[(2S)-2-[(3R)-3-(benzoylamino)-3-methyl-2,5-dioxo-1-pyrrolidinyl]-1-oxopropyl]-L-alanyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



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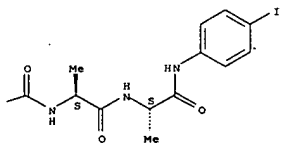

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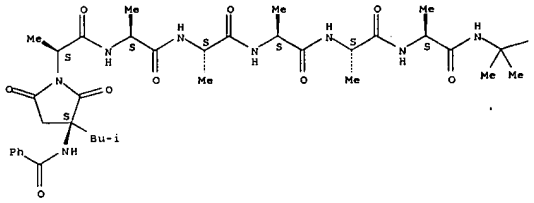
CN L-Alaninamide, N-[(2S)-2-[(3S)-3-(benzoylamino)-3-(2-methylpropyl)-2,5-dioxo-1-pyrrolidinyl]-1-oxopropyl]-L-alanyl-L-alanyl-L-alanyl-L-alanyl-L-alanyl-2-methylalanyl-L-alanyl-N-(4-iodophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



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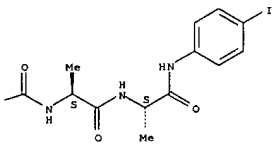

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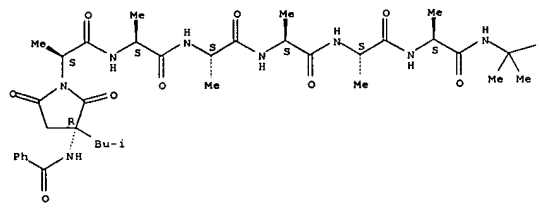
Absolute stereochemistry. Rotation (-).

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



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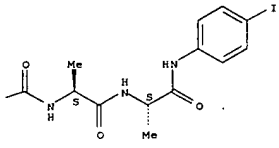

RN 197382-05-1 CAPLUS
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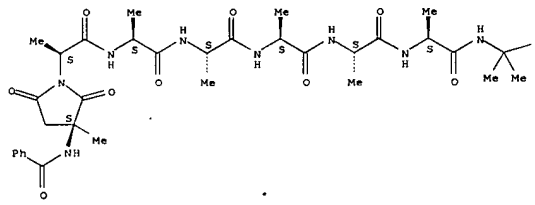
CM 1

CRN 197381-77-4
CMF C46 H62 I N11 O12

Absolute stereochemistry. Rotation (-).

L12 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

PAGE 1-A



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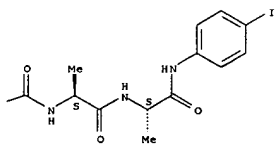


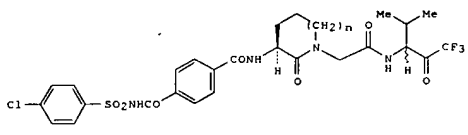
CM 2

CRN 75-05-8
CMF C2 H3 N

REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:135101 CAPLUS
DOCUMENT NUMBER: 120:135101
TITLE: Elastase inhibitors containing conformationally restricted lactams as P3-P2 dipeptide replacements
AUTHOR(S): Skiles, Jerry W.; Sorcek, Ronald; Jacober, Stephen; Miao, Clara; Mui, Philip W.; McNeil, Daniel; Rosenthal, Alan S.
CORPORATE SOURCE: Dep. Med. Chem., Boehringer Ingelheim Pharm., Inc., Ridgefield, CT, 06877, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1993), 3(4), 773-8
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:135101
GI



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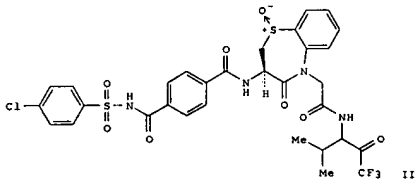
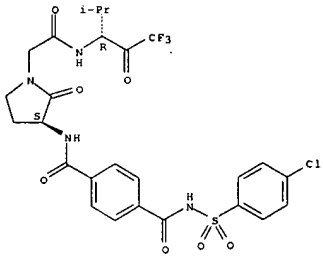


II

AB Title conformationally restricted lactams I (n = 0, 1, 2) and II were prepared as potential human leukocyte elastase (HLE) inhibitors.
IT 152839-11-7P 152839-12-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as human leukocyte elastase inhibitor)
RN 152839-11-7 CAPLUS
CN 1,4-Benzenedicarboxamide, N-[(4-chlorophenyl)sulfonyl]-N'-(2-oxo-1-[2-oxo-2-[[3,3,3-trifluoro-1-(1-methylethyl)-2-oxopropyl]amino]ethyl]-3-pyrrolidinyl]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

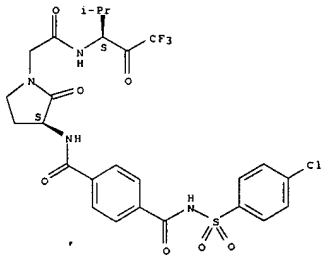
Absolute stereochemistry.

L12 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 152839-12-8 CAPLUS
CN 1,4-Benzenedicarboxamide, N-[(4-chlorophenyl)sulfonyl]-N'-[2-oxo-1-[2-oxo-2-[[3,3,3-trifluoro-1-(1-methylethyl)-2-oxopropyl]amino]ethyl]-3-pyrrolidinyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

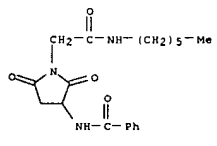
Absolute stereochemistry.



L12 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
at 0° followed by X. DL-BzNHCH(CH2CO2Et)CONHCH2CONH(CH2)5Me (XI), m. 105-7°, DL-BzNHCH(CO2Et)CH2CONHCH2CONH(CH2)5Me (XII), m. 82-7°, DL-BzNHCH(CH2CH2CO2Et)CONHCH2CONH(CH2)5Me (XIII), m. 110-12°, and L-PhCH2OCONHCH2CONHCH2CONHCH(CH2CH2CO2Et)CONHCH2CONH(CH2)5Me (XIV), m. 142-7°, [α]D18 3.6°, were thus prepd. The reaction between X and II with V yields DL-BzNHCH(CH2CO2H)CONHCH2CONH(CH2)5Me (XV), m. 179-80°, and DL-BzNHCH(CO2H)CH2CONHCH2CONH(CH2)5Me (XVI), m. 163-4°. XV was also obtained by refluxing XI with HCl and Me2CO. DL-BzNHCH(CH2CONH2)CONHCH2CONH(CH2)5Me (XVII), m. 186-7°, was prepd. from XV in a manner similar to the prepn. of IV. XVII is also obtained by treatment of XI with satd. alc. NH3. A soln. of XIV and AcOH in MeOH was shaken with H and Pd until CO2 evolution was complete. The filtered soln. was evapd. to a gum, the unreacted XIV removed, and the rest shaken with Ac2O. Evapn. gave a gum from which L-AcNHCH2CONHCH2CONHCH(CH2CH2CO2Et)CONHCH2CONH(CH2)5Me (XVIII), m. 193.5-4.5°, was isolated. XV, XVI and DL-benzamidosuccinoylglycine n-hexylamide, m. 149-50°, are obtained by the action of alkali on XI or XII, whereas BzNHCH(CO2H)CH2CH2CONHCH2CONH(CH2)5Me (XIX), m. 129-31°, and BzNHCH(CH2CH2CO2H)CONHCH2CONH(CH2)5Me (XX), m. 184-6°, are obtained from XIII. XVIII reacts with aq. NaOH to form L-AcNHCH2CONHCH2CONHCH(CH2CH2CO2H)CONHCH2CONH(CH2)5Me, m. 185-7°. XIX and XX were prepd. from X and N-benzoylglutamic anhydride, m. 154-5°, by the method used for the aspartyl analogs. The possible application of the observed rearrangements in a scheme for the specific fission of a peptide chain at the aspartic and glutamic residues are discussed.

IT 857423-00-8P, 1-Pyrrolidineacetamide, 3-benzamido-N-hexyl-2,5-dioxo-
RL: PREP (Preparation)
(preparation of)

RN 857423-00-8 CAPLUS
CN 1-Pyrrolidineacetamide, 3-benzamido-N-hexyl-2,5-dioxo- (9CI) (CA INDEX NAME)



L12 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1956:8140 CAPLUS
DOCUMENT NUMBER: 50:8140
ORIGINAL REFERENCE NO.: 50:1590h-i,1591a-h
TITLE: Studies on specific chemical fission of peptide links.
I. Rearrangements of aspartyl and glutamyl peptides
AUTHOR(S): Battersby, Alan R.; Robinson, J. C.
CORPORATE SOURCE: Univ. St. Andrews, UK
SOURCE: Journal of the Chemical Society (1955) 259-69
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

AB cf. C.A. 49, 864f. The esters of α- and β-aspartyl peptides, RCONHCH(CH2CO2Et)CONHR' and RCONHCH(CO2Et)CH2CONHR', are converted by alkaline hydrolysis into mixts. of aspartyl peptides, RCONHCH(CO2H)CH2CONHR' and RCONHCH(CH2CO2H)CONHR', the former product preponderating. DL-BzNHCH(CO2H)CH2CO2Et (I), m. 105-7°, was prepared from β-Et DL-aspartate-HCl, K2CO3 and BzCl; and DL-BzNHCH(CO2H)CH2CH2CO2Et, m. 114-15.5°, was prepared by benzoylation of γ-Et DL-glutamate. A stirred solution of I and Et3N (II) in dioxane and CHCl3 was treated at 0° with ClCO2Et (III), an excess of NH4OH added after 20 min., and the stirring continued for 5 hrs. After addition of water, the solution was acidified and concentrated, yielding DL-BzNHCH(CH2CO2Et)CONH2 (IV), m. 151-3°. The reaction between NH3 and N-benzoyl-DL-aspartic anhydride (V) yields DL-BzNHCH(CO2H)CH2CONH2 (VI), m. 189-90° and a small amount of DL-BzNHCH(CH2CO2H)CONH2 (VII), m. 208-9°. VI is also obtained from the reaction of I and dilute NH3, or upon the racemization of the L-amide. BzNHCH.CO.NH.CO.CH2 (VIII), m. 223-5°, prepared by the reaction of NaOH or NaOEt with IV, forms DL-BzNHCH(CONH2)CH2CONH2, m. 270°, upon treatment with NH4OH. DL-BzNHCH(CO2Et)CH2CO2Et (IX), m. 75-7°, was prepared by the reaction of the free acid with EtOH and dry HCl. Refluxing V with absolute EtOH yields IX, I, and DL-BzNHCH(CO2Et)CH2CO2H, m. 111-12.5°. DL-BzNHCH(CO2Et)CH2CONH2, m. 152-4°, was synthesized in a manner similar to IV. IV could not be cyclized by treatment with HBr in MeNO2 or HCl in EtOH. The action of alkali on IV or VIII yields mainly VI and a small amount of VII. n-C6H13NH2 in dioxane was added to a solution of phthaloylglycyl chloride and the solution concentrated Addition of 0.5% NaHCO3 gave a precipitate of phthaloylglycine n-hexylamide, m. 164-6°, which upon refluxing with N2H4.H2O followed by acidification gave Me(CH2)5NHCOCH2NH3Cl (X), m. 249°. A solution of benzyloxycarbonylglycylglycine and II in CHCl3 when treated at 0° with III followed by addition of γ-Et L-glutamate in 0.1N NaOH, yields PhCH2OCONHCH2CONHCH2CONHCH(CO2H)CH2CH2CO2Et, m. 151-3°. Me(CH2)5NHCOCH2NHCO2Et, m. 94-5°, was prepared from III, X, and II. Glycine n-hexylamides of acylaspartic and -glutamic acid monoesters can be prepared by the reaction of the monoester in dioxane-CHCl3 with II and III

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FULL ESTIMATED COST                                     44.95     397.81

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SESSION RESUMED IN FILE 'MEDLINE, CAPLUS' AT 10:45:46 ON 13 DEC 2006
FILE 'MEDLINE' ENTERED AT 10:45:46 ON 13 DEC 2006
FILE 'CAPLUS' ENTERED AT 10:45:46 ON 13 DEC 2006
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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
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FULL ESTIMATED COST                                     44.95     397.81

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CA SUBSCRIBER PRICE                                     -6.00      -6.00

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CA SUBSCRIBER PRICE                                     -6.00      -6.00

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DICTIONARY FILE UPDATES:  12 DEC 2006  HIGHEST RN 915277-53-1

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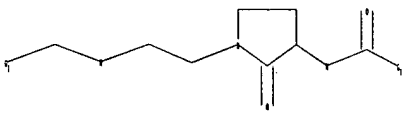

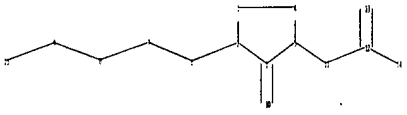

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ring nodes :
1 2 3 4 5
chain bonds :
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1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
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exact bonds :

10776586.trn

6-7

G1:Cb,Cy,Hy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
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L13 STRUCTURE UPLOADED

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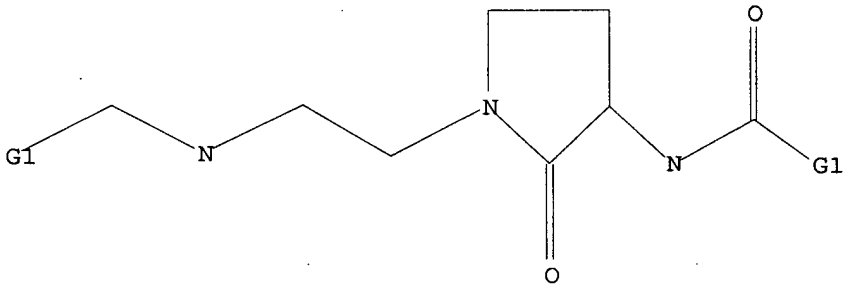
L13 STR




G1 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
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PROJECTED ANSWERS: 1 TO 80

L14 1 SEA SSS SAM L13

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SEARCH TIME: 00.00.01

L15 32 SEA SSS FUL L13

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FULL ESTIMATED COST                                   166.94     564.75

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=> l15
L16           3 L15

=> d his

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L2            50 L1
L3               STRUCTURE UPLOADED
L4            50 L3
L5           874 L3 FULL

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L6           300 L5
L7           284 DUP REM L6 (16 DUPLICATES REMOVED)

     FILE 'REGISTRY' ENTERED AT 10:28:07 ON 13 DEC 2006
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L9             1 L8
L10           23 L8 FULL

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L11            8 L10
L12            8 DUP REM L11 (0 DUPLICATES REMOVED)

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L13              STRUCTURE UPLOADED
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L15           32 L13 FULL

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=> l15 not l12
L17           2 L15 NOT L12

=> l16 not l12
L18           2 L16 NOT L12
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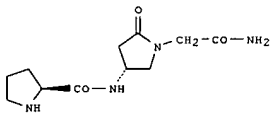
L18 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:645705 CAPLUS
DOCUMENT NUMBER: 140:87048
TITLE: iso-Lactam and reduced amide analogues of the peptidomimetic dopamine receptor modulator 3(R)-[(2(S)-pyrrolidinylcarbonyl)amino]-2-oxo-1-pyrrolidineacetamide
AUTHOR(S): Dolbeare, Kristine; Pontoriero, Giuseppe F.; Gupta, Suresh K.; Mishra, Ram K.; Johnson, Rodney L.
CORPORATE SOURCE: Department of Medicinal Chemistry, University of Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(18), 4103-4112
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:87048
GI



I

AB 4(R)-[[2(S)-pyrrolidinylcarbonyl]amino]-2-oxo-1-pyrrolidineacetamide (I), an analog of the title γ-lactam Pro-Leu-Gly-NH2 peptidomimetic and a series of other analogs were synthesized. The compds. were tested for their ability to enhance the binding of [3H]N-propylnorapomorphine to dopamine receptors in a functional in vitro assay utilizing bovine striatal membranes.

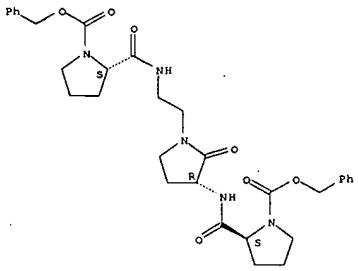
IT 644996-25-8P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of pyrrolidineacetamides as peptidomimetic dopamine receptor modulators)

RN 644996-25-8 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3R)-2-oxo-1-[2-[[[(2S)-1-[(phenylmethoxy)carbonyl]-2-pyrrolidinyl]carbonyl]amino]ethyl]-3-pyrrolidinyl]amino]carbonyl]-, phenylmethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L18 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1994:135143 CAPLUS
DOCUMENT NUMBER: 120:135143
TITLE: Preparation of peptides with tachykinin antagonist activity
INVENTOR(S): Matsuo, Masaaki; Hagiwara, Daijiro; Miyake, Hiroishi; Igari, Norihiro; Murano, Kenji
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 9314113 | A1 | 19930722 | WO 1993-JP2 | 19930104 |
| W: CA, JP, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| EP 620824 | A1 | 19941026 | EP 1993-900452 | 19930104 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE | | | | |
| JP 07503711 | T2 | 19950420 | JP 1993-512326 | 19930104 |

PRIORITY APPLN. INFO.: GB 1992-535 A 19920110
WO 1993-JP2 W 19930104

OTHER SOURCE(S): MARPAT 120:135143
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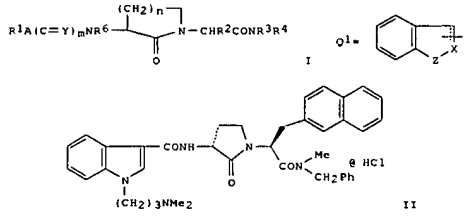


I



II

AB Title compds. [I; R1 = (substituted) aryl, pyridyl, pyrrolyl, Q1; dotted line = optional double bond; X = CH, N; Z = O, S, NH; R2, R4 = (substituted) aralkyl; R3 = (substituted) alkyl; R6 = H, alkyl; A = bond, alkylene, alkenylene; Y = O, NR7; R7 = H, alkyl; m = 0, 1; n = 0, 2], were prepared Thus, title compound II, prepared by solution phase methods, at 10 mg/kg orally in guinea pigs gave 95.7% inhibition of substance P-induced bronchoedema.

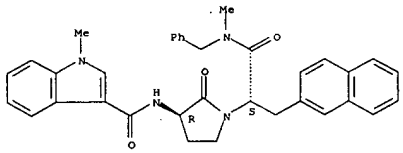
L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

IT 153050-31-8P 153050-32-9P 153050-33-0P
153050-34-1P 153050-35-2P 153050-36-3P
153050-37-4P 153050-38-5P 153050-40-9P
153050-41-0P 153050-42-1P 153050-43-2P
153050-44-3P 153050-45-4P 153050-46-5P
153050-47-6P 153050-48-7P 153050-50-1P
153050-51-2P 153050-52-3P 153050-53-4P
153050-55-6P 153050-56-7P 153090-78-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as tachykinin antagonist)

RN 153050-31-8 CAPLUS

CN 1H-Indole-3-carboxamide, 1-methyl-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

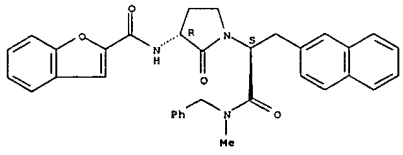
Absolute stereochemistry.



RN 153050-32-9 CAPLUS

CN 1-Pyrrolidineacetamide, 3-[(2-benzofuranylcarbonyl)amino]-N-methyl-α-(2-naphthalenylmethyl)-2-oxo-N-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

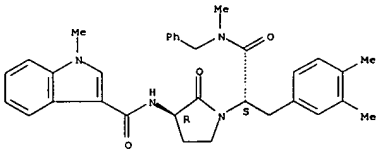


RN 153050-33-0 CAPLUS

CN 1H-Indole-3-carboxamide, N-[1-[1-[(3,4-dimethylphenyl)methyl]-2-[methyl(phenylmethyl)amino]-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-1-methyl-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

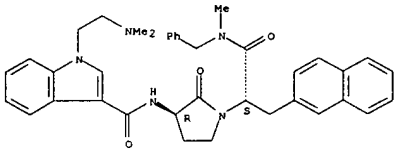
L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



RN 153050-34-1 CAPLUS
CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

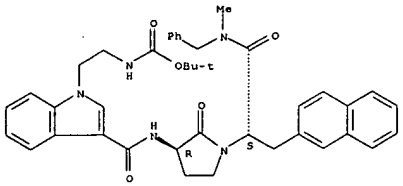
Absolute stereochemistry.



RN 153050-35-2 CAPLUS
CN Carbamic acid, [2-[3-[[[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]amino]carbonyl]-1H-indol-1-yl]ethyl]-, 1,1-dimethylethyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

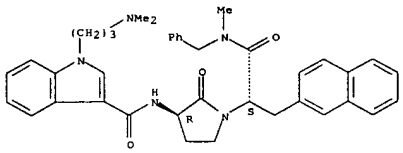
Absolute stereochemistry.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



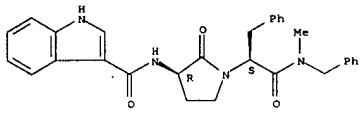
RN 153050-36-3 CAPLUS
CN 1H-Indole-3-carboxamide, 1-[3-(dimethylamino)propyl]-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153050-37-4 CAPLUS
CN 1H-Indole-3-carboxamide, N-[1-[2-[methyl(phenylmethyl)amino]-2-oxo-1-(phenylmethyl)ethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

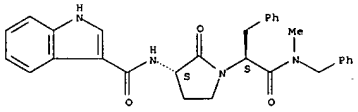


RN 153050-38-5 CAPLUS

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

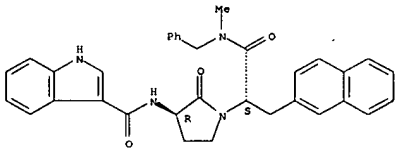
CN 1H-Indole-3-carboxamide, N-[1-[2-[methyl(phenylmethyl)amino]-2-oxo-1-(phenylmethyl)ethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153050-40-9 CAPLUS
CN 1H-Indole-3-carboxamide, N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

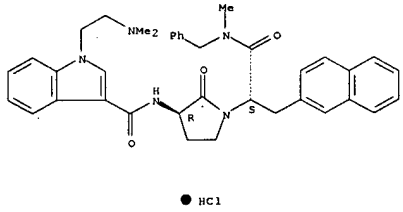
Absolute stereochemistry.



RN 153050-41-0 CAPLUS
CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

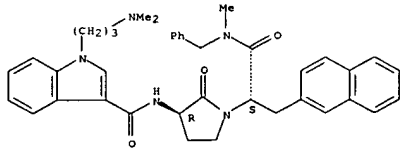
L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● HCl

RN 153050-42-1 CAPLUS
CN 1H-Indole-3-carboxamide, 1-[3-(dimethylamino)propyl]-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

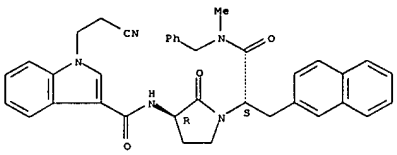


● HCl

RN 153050-43-2 CAPLUS
CN 1H-Indole-3-carboxamide, 1-(2-cyanoethyl)-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

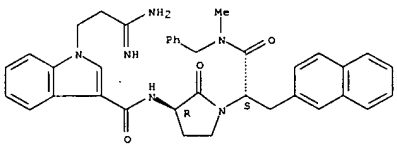
Absolute stereochemistry.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 153050-44-3 CAPLUS
CN 1H-Indole-3-carboxamide, 1-(3-amino-3-iminopropyl)-3-[[[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]amino]carbonyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

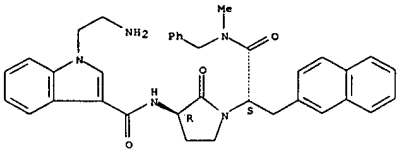


● HCl

RN 153050-45-4 CAPLUS
CN 1H-Indole-3-carboxamide, 1-(2-aminoethyl)-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

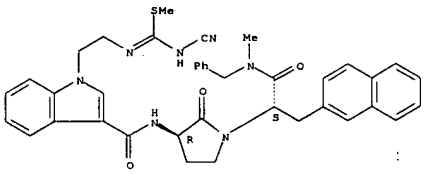
L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



● HCl

RN 153050-46-5 CAPLUS
CN Carbamimidothioic acid, N-cyano-N'-[2-[3-[[[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]amino]carbonyl]-1H-indol-1-yl]ethyl]-, methyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

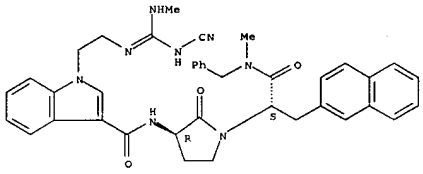
Absolute stereochemistry.
Double bond geometry unknown.



RN 153050-47-6 CAPLUS
CN 1H-Indole-3-carboxamide, 1-[2-[[(cyanoamino)(methylamino)methylene]amino]ethyl]-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

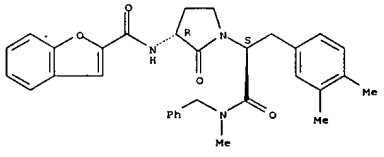
Absolute stereochemistry.
Double bond geometry unknown.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



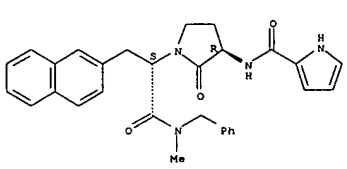
RN 153050-48-7 CAPLUS
CN 1-Pyrrolidineacetamide, 3-[(2-benzofuranylcarbonyl)amino]-α-[(3,4-dimethylphenyl)methyl]-N-methyl-2-oxo-N-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153050-50-1 CAPLUS
CN 1H-Pyrrole-2-carboxamide, N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI)
(CA INDEX NAME)

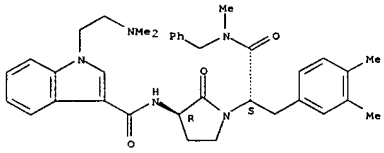
Absolute stereochemistry.



RN 153050-51-2 CAPLUS
CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-[1-[1-[(3,4-dimethylphenyl)methyl]-2-[methyl(phenylmethyl)amino]-2-oxoethyl]-2-oxo-3-

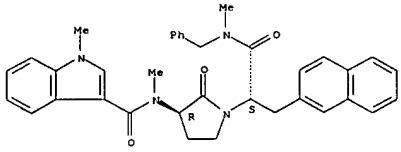
L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



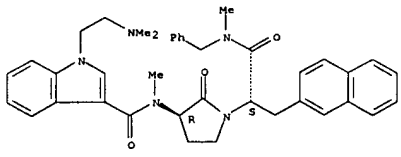
RN 153050-52-3 CAPLUS
CN 1H-Indole-3-carboxamide, N,1-dimethyl-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153050-53-4 CAPLUS
CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-methyl-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

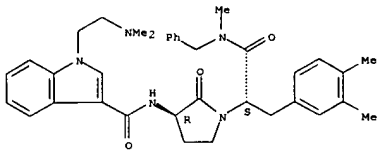
Absolute stereochemistry.



RN 153050-55-6 CAPLUS

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-[1-[1-[(3,4-dimethylphenyl)methyl]-2-[methyl(phenylmethyl)amino]-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

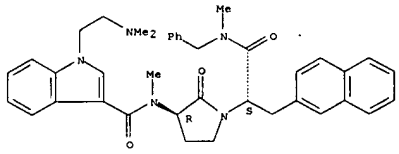
Absolute stereochemistry.



● HCl

RN 153050-56-7 CAPLUS
CN 1H-Indole-3-carboxamide, 1-[2-(dimethylamino)ethyl]-N-methyl-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, monohydrochloride, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

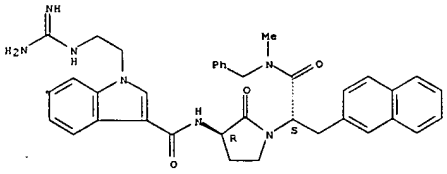


● HCl

RN 153090-78-9 CAPLUS
CN 1H-Indole-3-carboxamide, 1-[2-[(aminoiminomethyl)amino]ethyl]-N-[1-[2-[methyl(phenylmethyl)amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]-2-oxo-3-pyrrolidinyl]-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L18 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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STRUCTURE FILE UPDATES:   12 DEC 2006  HIGHEST RN 915277-53-1
DICTIONARY FILE UPDATES:  12 DEC 2006  HIGHEST RN 915277-53-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

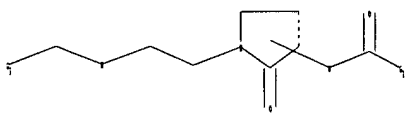
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

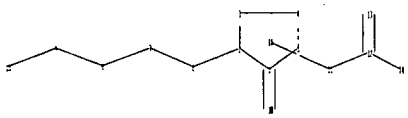
  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 5.str
```





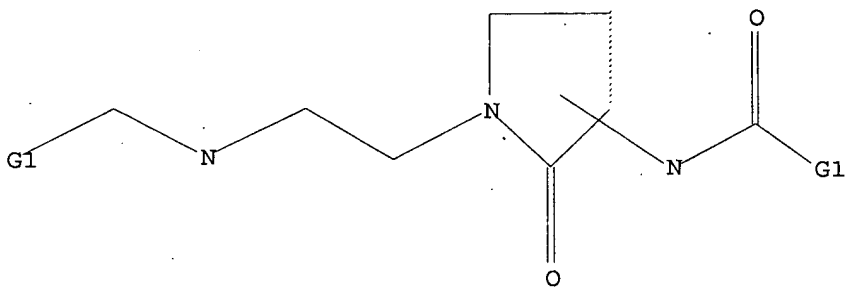
chain nodes :
6 7 8 9 10 11 12 13 14 15
ring nodes :
1 2 3 4 5
chain bonds :
1-10 2-6 6-7 7-8 8-9 9-15 11-12 12-13 12-14
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-10 2-3 2-6 3-4 4-5 7-8 8-9 9-15 11-12 12-13 12-14
exact bonds :
6-7

G1:Cb,Cy,Hy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 18:CLASS

L19 STRUCTURE UPLOADED

```
=> d
L19 HAS NO ANSWERS
L19              STR
```




```
G1 Cb,Cy,Hy


Structure attributes must be viewed using STN Express query preparation.


=> l19
SAMPLE SEARCH INITIATED 10:51:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     2466 TO ITERATE

 81.1% PROCESSED     2000 ITERATIONS                                 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        46342 TO    52298
PROJECTED ANSWERS:               0 TO        0

L20            0 SEA SSS SAM L19

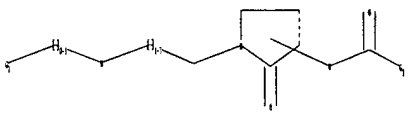
=> l19 full
FULL SEARCH INITIATED 10:51:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    49992 TO ITERATE

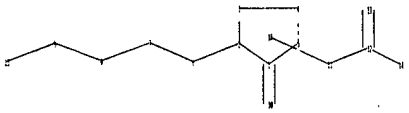
100.0% PROCESSED    49992 ITERATIONS                               32 ANSWERS
SEARCH TIME: 00.00.01

L21           32 SEA SSS FUL L19

=> l21 not l15
L22            0 L21 NOT L15

=>
Uploading C:\Program Files\Stnexp\Queries\10776586\Struc 6.str
```





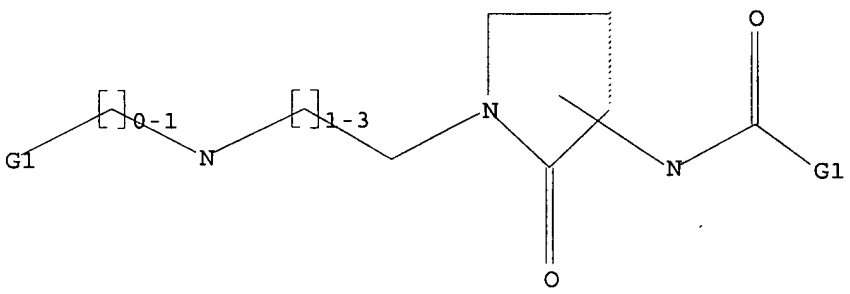
chain nodes :
6 7 8 9 10 11 12 13 14 15
ring nodes :
1 2 3 4 5
chain bonds :
1-10 2-6 6-7 7-8 8-9 9-15 11-12 12-13 12-14
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-10 2-3 2-6 3-4 4-5 7-8 8-9 9-15 11-12 12-13 12-14
exact bonds :
6-7

G1:Cb,Cy,Hy

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 18:CLASS

L23 STRUCTURE UPLOADED

```
=> d
L23 HAS NO ANSWERS
L23             STR
```




```
G1 Cb,Cy,Hy


Structure attributes must be viewed using STN Express query preparation.


=> l23
SAMPLE SEARCH INITIATED 10:53:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     5114 TO ITERATE

 39.1% PROCESSED     2000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        97992 TO   106568
PROJECTED ANSWERS:               0 TO        0

L24           0 SEA SSS SAM L23

=> l23 full
FULL SEARCH INITIATED 10:54:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   104500 TO ITERATE

100.0% PROCESSED   104500 ITERATIONS                               42 ANSWERS
SEARCH TIME: 00.00.04

L25          42 SEA SSS FUL L23

=> file medline caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   335.20     915.31

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -7.50

FILE 'MEDLINE' ENTERED AT 10:54:14 ON 13 DEC 2006

FILE 'CAPLUS' ENTERED AT 10:54:14 ON 13 DEC 2006
```

```
=> l25
L26           5 L25

=> d his

     (FILE 'HOME' ENTERED AT 10:26:24 ON 13 DEC 2006)

     FILE 'REGISTRY' ENTERED AT 10:26:36 ON 13 DEC 2006
L1               STRUCTURE UPLOADED
L2            50 L1
L3               STRUCTURE UPLOADED
L4            50 L3
L5           874 L3 FULL

     FILE 'MEDLINE, CAPLUS' ENTERED AT 10:27:48 ON 13 DEC 2006
L6           300 L5
L7           284 DUP REM L6 (16 DUPLICATES REMOVED)

     FILE 'REGISTRY' ENTERED AT 10:28:07 ON 13 DEC 2006
L8               STRUCTURE UPLOADED
L9             1 L8
L10           23 L8 FULL

     FILE 'MEDLINE, CAPLUS' ENTERED AT 10:28:52 ON 13 DEC 2006
L11            8 L10
L12            8 DUP REM L11 (0 DUPLICATES REMOVED)

     FILE 'REGISTRY' ENTERED AT 10:45:52 ON 13 DEC 2006
L13              STRUCTURE UPLOADED
L14            1 L13
L15           32 L13 FULL

     FILE 'MEDLINE, CAPLUS' ENTERED AT 10:46:20 ON 13 DEC 2006
L16            3 L15
L17            2 L15 NOT L12
L18            2 L16 NOT L12

     FILE 'REGISTRY' ENTERED AT 10:51:21 ON 13 DEC 2006
L19              STRUCTURE UPLOADED
L20            0 L19
L21           32 L19 FULL
L22            0 L21 NOT L15
L23              STRUCTURE UPLOADED
L24            0 L23
L25           42 L23 FULL

     FILE 'MEDLINE, CAPLUS' ENTERED AT 10:54:14 ON 13 DEC 2006
L26            5 L25

=> l26 not l12
L27            4 L26 NOT L12

=> l27 not l18
```

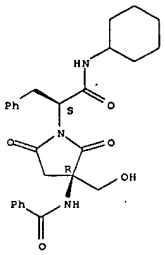
L28 2 L27 NOT L18

=> d ibib abs hitstr 1-2

L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:516307 CAPLUS
DOCUMENT NUMBER: 125:276500
TITLE: Synthesis, conformational properties, and synthetic applications of novel optically pure α,α-disubstituted (R)- and (S)-glycines (α chimeras) combining side chains of Asp, Glu, Leu, Phe, Ser, and Val
AUTHOR(S): Obrecht, Daniel; Abrecht, Christine; Altorfer, Michael; Bohdal, Udo; Grieder, Alfred; Kleber, Martina; Pfyffer, Patrick; Mueller, Klaus
CORPORATE SOURCE: Hoffmann-La Roche A.-G., Basel, CH-4002, Switz.
SOURCE: Helvetica Chimica Acta (1996), 79(5), 1315-1337
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of novel open-chain and cyclic conformationally constrained α,α-disubstituted (R)- and (S)-glycine derivs. (α-chimeras) combining side chains of Asp, Glu, Leu, Phe, Ser, and Val were efficiently prepared by α-alkylation of racemic 4-monosubstituted 2-phenyl-1,3-oxazol-5(4H)-ones, resolution after reaction with (S)-phenylalanine cyclohexylamide as chiral auxiliary, a novel azolactone/dihydrooxazole interconversion reaction to synthesize optically pure α-substituted (R) and (S)-serine derivs. coupled with succinimide-ring formation of aspartic acid derivs. Based on x-ray structures, the absolute configuration of these novel amino-acid building blocks was unambiguously determined and their preferred conformations in the crystalline state were assessed.
IT 182176-33-6P 182268-07-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (CD spectra; synthesis, conformation, and synthetic applications of α,α-disubstituted glycines)
RN 182176-33-6 CAPLUS
CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-(hydroxymethyl)-2,5-dioxo-α-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

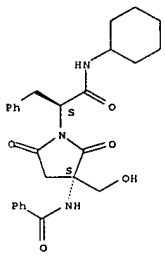
Absolute stereochemistry.

L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 182268-07-1 CAPLUS
CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-(hydroxymethyl)-2,5-dioxo-α-(phenylmethyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

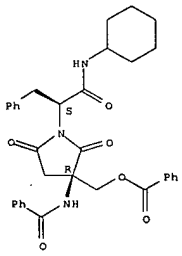
Absolute stereochemistry.



IT 182176-31-4P 182176-36-9P 182268-06-0P
182268-08-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis, conformation, and synthetic applications of α,α-disubstituted glycines)
RN 182176-31-4 CAPLUS
CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-3-[(benzoyloxy)methyl]-N-cyclohexyl-2,5-dioxo-α-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

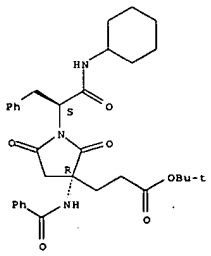
Absolute stereochemistry.

L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 182176-36-9 CAPLUS
CN 3-Pyrrolidinepropanoic acid, 3-(benzoylamino)-1-[2-(cyclohexylamino)-2-oxo-1-(phenylmethyl)ethyl]-2,5-dioxo-, 1,1-dimethylethyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

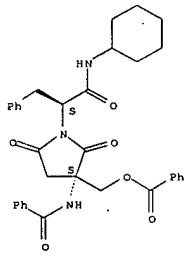
Absolute stereochemistry.



RN 182268-06-0 CAPLUS
CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-3-[(benzoyloxy)methyl]-N-cyclohexyl-2,5-dioxo-α-(phenylmethyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

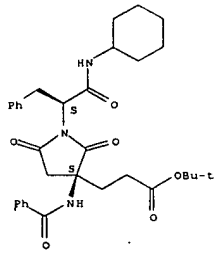
Absolute stereochemistry.

L28 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

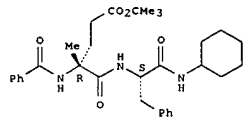


RN 182268-08-2 CAPLUS
CN 3-Pyrrolidinepropanoic acid, 3-(benzoylamino)-1-[2-(cyclohexylamino)-2-oxo-1-(phenylmethyl)ethyl]-2,5-dioxo-, 1,1-dimethylethyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

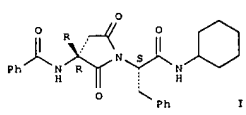
Absolute stereochemistry.



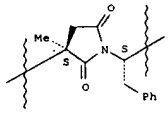
L28 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:842202 CAPLUS
DOCUMENT NUMBER: 124:56605
TITLE: A novel synthesis of (R)- and (S)-α-alkylated aspartic and glutamic acids: α-alkylated aspartic succinimides as new type of β-turn type II and II' mimetics
AUTHOR(S): Obrecht, Daniel; Bohdal, Udo; Daly, John; Lehmann, Christian; Schoenholzer, Peter; Mueller, Klaus
CORPORATE SOURCE: Pharma Res., F. Hoffmann-La Roche AG, Basel, CH-4002, Switz.
SOURCE: Tetrahedron (1995), 51(40), 10883-900
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:56605
GI



I



II

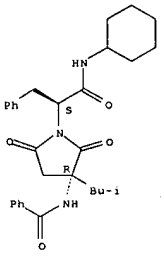


III

AB A novel and efficient synthesis of optically pure (R)- and (S)-α-methylglutamic acid, (R)- and (S)-α-methylaspartic acid, and (R)- and (S)-α-isobutylaspartic acid, using L-phenylalanine cyclohexylamide as chiral auxiliary, is described. Crystal structures show that the (R)- (I) (R,S-configuration) and (S)-α-methylglutamic acid derivs. adopt β-turn type I geometries, whereas the corresponding aspartimide derivs. II (R = Me, isobutyl) (R,S) form a β-turn type II and III (S,S) a β-turn type II'. These findings suggest that the succinimide derivs. of (R)- and (S)-α-alkylaspartic acids can serve as building blocks to stabilize β-turns of type II (or II') in peptides, depending on their absolute configuration.
IT 172095-19-1P 172275-38-6P 172275-39-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and conformation of alkylated aspartic and glutamic acids and aspartic succinimide derivs.)

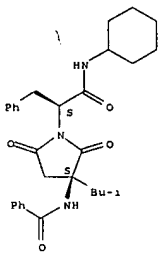
L28 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



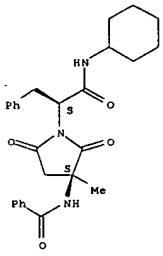
IT 172095-20-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and conformation of alkylated aspartic and glutamic acids and aspartic succinimide derivs.)
RN 172095-20-4 CAPLUS
CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-(2-methylpropyl)-2,5-dioxo-α-(phenylmethyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



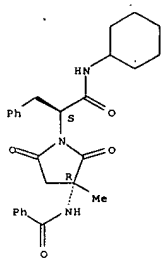
L28 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 172095-19-1 CAPLUS
CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-methyl-2,5-dioxo-α-(phenylmethyl)-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 172275-38-6 CAPLUS
CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-methyl-2,5-dioxo-α-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 172275-39-7 CAPLUS
CN 1-Pyrrolidineacetamide, 3-(benzoylamino)-N-cyclohexyl-3-(2-methylpropyl)-2,5-dioxo-α-(phenylmethyl)-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

```
=> log h
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                   11.91     927.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -1.50      -9.00

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:55:15 ON 13 DEC 2006
```